



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:36 PM GMT

PDB ID : 1ZZ2  
Title : Two Classes of p38alpha MAP Kinase Inhibitors Having a Common Diphenylether Core but Exhibiting Divergent Binding Modes  
Authors : Michelotti, E.L.; Moffett, K.K.; Springman, E.B.; Karpusas, M.  
Deposited on : 2005-06-13  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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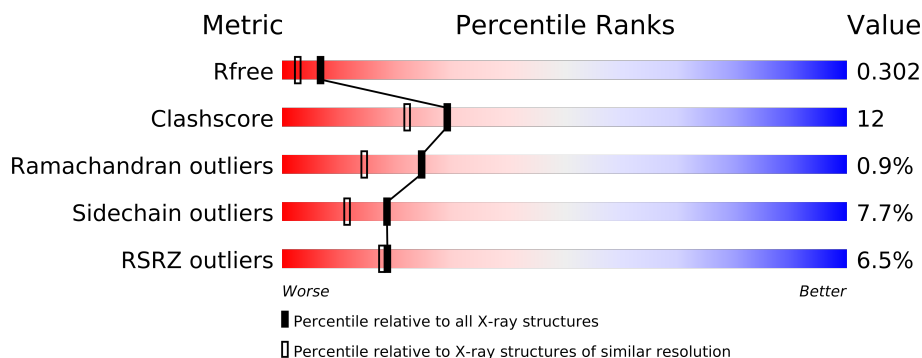
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	360	

## 2 Entry composition i

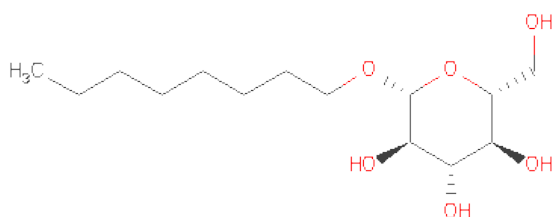
There are 4 unique types of molecules in this entry. The entry contains 2872 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

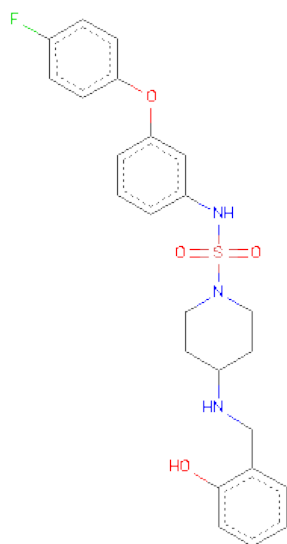
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2716	1744	464	496	12	5	0	0

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	20	14	6	0	0

- Molecule 3 is N-[3-(4-FLUOROPHENOXY)PHENYL]-4-[(2-HYDROXYBENZYL)AMINO] PIPERIDINE-1-SULFONAMIDE (three-letter code: B11) (formula: C<sub>24</sub>H<sub>26</sub>FN<sub>3</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	33	24	1	3	4	1	1	0

- Molecule 4 is water.

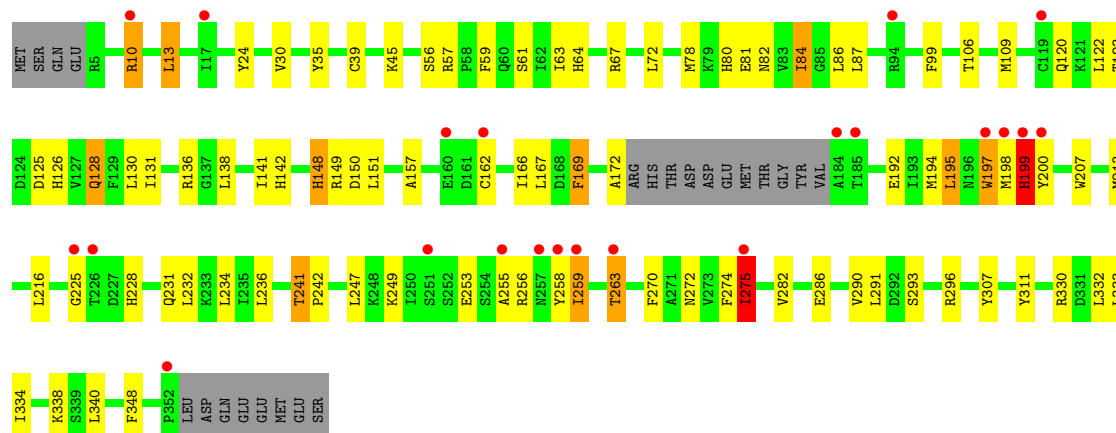
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Mitogen-activated protein kinase 14

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.29Å 74.23Å 74.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.00 48.60 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.00) 87.0 (48.60-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.256 , 0.290 0.268 , 0.302	Depositor DCC
$R_{free}$ test set	2830 reflections (8.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 29.8	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 37948 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B11, BOG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	1/2779 (0.0%)	0.60	0/3773

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	CYS	CB-SG	7.91	1.95	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	HIS	Sidechain
1	A	169	PHE	Sidechain
1	A	199	HIS	Sidechain
1	A	200	TYR	Sidechain
1	A	24	TYR	Sidechain
1	A	258	TYR	Sidechain
1	A	30	VAL	Peptide
1	A	307	TYR	Sidechain
1	A	311	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	348	PHE	Sidechain
1	A	35	TYR	Sidechain
1	A	99	PHE	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2716	0	2721	67	0
2	A	20	0	21	9	0
3	A	33	0	25	1	0
4	A	103	0	0	3	0
All	All	2872	0	2767	68	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (68) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:LEU:HB3	1:A:263:THR:HG23	1.41	1.02
1:A:259:ILE:HG13	2:A:361:BOG:H8'2	1.61	0.81
1:A:148:HIS:HD2	1:A:150:ASP:H	1.33	0.77
1:A:80:HIS:HD2	1:A:82:ASN:H	1.32	0.76
1:A:192:GLU:HB3	2:A:361:BOG:H3'1	1.74	0.69
1:A:80:HIS:CD2	1:A:82:ASN:H	2.10	0.68
1:A:81:GLU:HG3	1:A:136:ARG:HH12	1.61	0.65
1:A:242:PRO:HG2	1:A:259:ILE:HD12	1.80	0.63
1:A:259:ILE:HD13	1:A:259:ILE:O	1.98	0.63
1:A:291:LEU:O	2:A:361:BOG:H2'2	1.98	0.63
1:A:149:ARG:HD2	1:A:172:ALA:O	1.99	0.63
1:A:197:TRP:CH2	1:A:255:ALA:HB1	2.35	0.62
1:A:84:ILE:HG22	1:A:166:ILE:O	1.99	0.61
1:A:195:LEU:HD13	1:A:232:LEU:HD21	1.82	0.60
1:A:148:HIS:CD2	1:A:150:ASP:H	2.19	0.59
1:A:259:ILE:HG13	2:A:361:BOG:C8'	2.32	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:ARG:H	1:A:10:ARG:HE	1.50	0.59
1:A:282:VAL:O	1:A:286:GLU:HG3	2.03	0.58
1:A:148:HIS:HE1	1:A:167:LEU:O	1.87	0.58
1:A:59:PHE:CD2	1:A:338:LYS:HE2	2.39	0.57
1:A:290:VAL:O	1:A:296:ARG:HD2	2.05	0.57
1:A:63:ILE:O	1:A:67:ARG:HG2	2.05	0.57
1:A:293:SER:OG	2:A:361:BOG:H1	2.04	0.56
1:A:13:LEU:HD23	1:A:39:CYS:SG	2.48	0.53
1:A:236:LEU:HD21	1:A:259:ILE:HD11	1.90	0.53
1:A:81:GLU:CG	1:A:136:ARG:HH12	2.20	0.53
1:A:241:THR:HA	1:A:263:THR:HG21	1.91	0.51
1:A:148:HIS:HD2	1:A:150:ASP:N	2.07	0.50
1:A:10:ARG:N	1:A:10:ARG:HE	2.09	0.50
1:A:141:ILE:HG13	1:A:142:HIS:N	2.25	0.50
1:A:84:ILE:HD11	3:A:362:B11:C29	2.43	0.49
1:A:195:LEU:HD13	1:A:232:LEU:CD2	2.43	0.49
1:A:272:ASN:O	1:A:275:ILE:HG13	2.12	0.48
1:A:84:ILE:HG13	1:A:106:THR:OG1	2.14	0.48
1:A:234:LEU:HB3	4:A:384:HOH:O	2.14	0.48
1:A:84:ILE:HG23	1:A:169:PHE:HE2	1.79	0.47
1:A:207:TRP:HA	4:A:412:HOH:O	2.14	0.47
1:A:78:MET:HG3	1:A:169:PHE:CZ	2.49	0.47
1:A:256:ARG:O	1:A:259:ILE:HG22	2.15	0.46
1:A:61:SER:HA	1:A:334:ILE:HD11	1.97	0.46
1:A:123:THR:H	1:A:126:HIS:CD2	2.34	0.45
1:A:290:VAL:O	1:A:296:ARG:CD	2.64	0.45
1:A:330:ARG:HG3	1:A:332:LEU:HD21	1.99	0.45
1:A:330:ARG:CG	1:A:332:LEU:HD21	2.47	0.45
1:A:270:PHE:CD1	1:A:286:GLU:HG2	2.51	0.45
1:A:57:ARG:O	1:A:64:HIS:HD2	2.00	0.45
1:A:148:HIS:O	1:A:149:ARG:HG2	2.18	0.44
1:A:242:PRO:HB2	1:A:247:LEU:HD21	1.99	0.44
1:A:249:LYS:HE2	2:A:361:BOG:O2	2.16	0.44
1:A:45:LYS:HE2	1:A:45:LYS:HB3	1.89	0.44
1:A:199:HIS:O	2:A:361:BOG:H61	2.17	0.44
1:A:242:PRO:HA	4:A:433:HOH:O	2.16	0.44
1:A:195:LEU:HG	1:A:197:TRP:CZ3	2.52	0.44
1:A:131:ILE:HG21	1:A:213:MET:HE3	2.00	0.44
1:A:125:ASP:HA	1:A:128:GLN:HG3	2.00	0.43
1:A:259:ILE:HD13	1:A:259:ILE:C	2.38	0.43
1:A:225:GLY:HA3	1:A:231:GLN:HB2	2.00	0.43
1:A:148:HIS:CE1	1:A:167:LEU:O	2.71	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:THR:HG22	1:A:125:ASP:H	1.84	0.42
1:A:84:ILE:CG2	1:A:169:PHE:HE2	2.32	0.42
1:A:109:MET:HB2	1:A:157:ALA:HB1	2.01	0.42
1:A:122:LEU:HD12	1:A:216:LEU:HD22	2.01	0.41
1:A:195:LEU:HG	1:A:197:TRP:CH2	2.55	0.41
1:A:197:TRP:CD1	2:A:361:BOG:H3'2	2.55	0.41
1:A:242:PRO:CG	1:A:259:ILE:HD12	2.48	0.41
1:A:274:PHE:O	1:A:275:ILE:C	2.58	0.41
2:A:361:BOG:H4'1	2:A:361:BOG:H7'1	1.81	0.40
1:A:242:PRO:HB2	1:A:247:LEU:CD2	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/360 (92%)	320 (96%)	10 (3%)	3 (1%)	25 14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	199	HIS
1	A	275	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/320 (93%)	275 (92%)	23 (8%)	18	11

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	13	LEU
1	A	72	LEU
1	A	84	ILE
1	A	86	LEU
1	A	87	LEU
1	A	120	GLN
1	A	128	GLN
1	A	130	LEU
1	A	138	LEU
1	A	151	LEU
1	A	194	MET
1	A	195	LEU
1	A	197	TRP
1	A	198	MET
1	A	228	HIS
1	A	241	THR
1	A	253	GLU
1	A	259	ILE
1	A	263	THR
1	A	275	ILE
1	A	333	LEU
1	A	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	64	HIS
1	A	80	HIS
1	A	120	GLN
1	A	126	HIS
1	A	148	HIS
1	A	269	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	BOG	A	361	-	20,20,20	3.19	4 (20%)	25,25,25	3.08	11 (44%)
3	B11	A	362	-	36,36,36	7.83	26 (72%)	50,50,50	1.69	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	A	361	-	5/5/5/5	0/11/31/31	0/1/1/1
3	B11	A	362	-	-	0/20/30/30	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	362	B11	O18-S16	30.41	1.73	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	362	B11	O19-S16	29.33	1.72	1.42
3	A	362	B11	S16-N17	8.33	1.73	1.63
2	A	361	BOG	O2-C2	-8.15	1.23	1.43
2	A	361	BOG	O3-C3	-8.05	1.23	1.43
2	A	361	BOG	O4-C4	-7.96	1.23	1.43
3	A	362	B11	S16-N13	6.44	1.78	1.62
3	A	362	B11	O7-C6	-5.91	1.24	1.36
3	A	362	B11	F1-C30	5.66	1.49	1.36
3	A	362	B11	C31-C30	4.85	1.46	1.36
3	A	362	B11	C29-C30	4.60	1.45	1.36
3	A	362	B11	C6-C5	3.88	1.45	1.39
3	A	362	B11	C21-C20	3.81	1.46	1.39
3	A	362	B11	C32-C31	3.81	1.46	1.38
3	A	362	B11	C29-C28	3.74	1.45	1.38
3	A	362	B11	C25-C20	3.68	1.45	1.39
3	A	362	B11	C21-C22	3.66	1.45	1.38
3	A	362	B11	C32-C27	3.61	1.46	1.38
3	A	362	B11	C4-C5	3.48	1.45	1.39
3	A	362	B11	C23-C22	3.47	1.45	1.38
3	A	362	B11	C28-C27	3.40	1.45	1.38
3	A	362	B11	C1-C6	3.32	1.45	1.39
3	A	362	B11	C2-C1	3.07	1.46	1.39
3	A	362	B11	C3-C2	3.00	1.46	1.37
3	A	362	B11	C3-C4	2.96	1.45	1.39
3	A	362	B11	C24-C25	2.88	1.45	1.39
3	A	362	B11	C24-C23	2.79	1.45	1.39
3	A	362	B11	O26-C27	-2.32	1.34	1.39
3	A	362	B11	O26-C22	-2.27	1.34	1.39
2	A	361	BOG	O6-C6	-2.18	1.32	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	BOG	O1-C1-C2	5.66	115.39	108.18
2	A	361	BOG	O2-C2-C1	5.39	121.80	110.04
2	A	361	BOG	C3-C4-C5	4.95	119.03	110.20
2	A	361	BOG	O3-C3-C4	4.66	120.80	110.35
2	A	361	BOG	O3-C3-C2	4.65	120.77	110.35
3	A	362	B11	O19-S16-O18	-4.63	113.11	119.46
2	A	361	BOG	O2-C2-C3	4.56	120.57	110.35
2	A	361	BOG	O4-C4-C5	4.50	121.14	109.28
2	A	361	BOG	O4-C4-C3	4.22	119.83	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	BOG	C4-C3-C2	4.12	118.43	110.82
2	A	361	BOG	C1-C2-C3	3.92	117.63	110.00
3	A	362	B11	C8-C5-C6	-3.80	115.40	120.21
3	A	362	B11	C4-C5-C6	3.59	122.49	118.16
3	A	362	B11	C25-C20-N17	-3.54	112.21	120.07
3	A	362	B11	C25-C20-C21	3.37	123.60	119.66
3	A	362	B11	N17-S16-N13	3.17	112.93	105.96
2	A	361	BOG	C1-O5-C5	2.64	118.86	113.73
3	A	362	B11	C3-C4-C5	-2.29	117.29	120.90
3	A	362	B11	C28-C29-C30	2.18	120.64	118.33

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	361	BOG	C4
2	A	361	BOG	C3
2	A	361	BOG	C1
2	A	361	BOG	C2
2	A	361	BOG	C5

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	337/360 (93%)	0.12	22 (6%) 18 18	12, 24, 55, 71	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	MET	8.5
1	A	184	ALA	6.8
1	A	197	TRP	4.7
1	A	185	THR	4.4
1	A	352	PRO	3.9
1	A	199	HIS	3.6
1	A	275	ILE	3.4
1	A	160	GLU	3.3
1	A	10	ARG	3.2
1	A	259	ILE	3.1
1	A	263	THR	2.8
1	A	258	TYR	2.7
1	A	94	ARG	2.7
1	A	200	TYR	2.7
1	A	251	SER	2.6
1	A	255	ALA	2.6
1	A	257	ASN	2.6
1	A	17	ILE	2.5
1	A	226	THR	2.4
1	A	119	CYS	2.1
1	A	225	GLY	2.1
1	A	162	CYS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BOG	A	361	20/20	0.35	1.24	59,61,64,64	0
3	B11	A	362	33/33	0.10	-0.22	19,21,22,23	1

### 6.5 Other polymers

There are no such residues in this entry.